



Development of New Electrolytes for Lithium-Sulfur Batteries

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US DOE VTO Annual Merit Review, Washington DC, June 21-23, 2022

Project ID: bat423

Overview and Relevance

This research work aims to develop new electrolytes and additives to enable sulfur as a high capacity and long cycle-life material for positive electrode and lithium metal as a negative electrode, to address three of the barriers of energy storage device for EV/PHEV application, insufficient energy density, poor cycle life performance, and poor calendar life.

Timeline	Budget	Barriers Addressed
Project started: FY2021	Total project funding	Performance: Low energy density
Project end date: FY2023	DOE share: \$1,350K, 100%	Life: Poor cycle and calendar life
Percent complete: 50%	FY22 funding \$450K	Cost: High materials and cell cost
	FY23 planned funding \$450K	
Partners		
LBNL (Dr. Chenhui Zhu, Dr. Jinghua Guo and Dr. Wanli Yang,)		
UC Berkeley (Prof. Andrew Minor)		
General Motors (Dr. Mei Cai)		
Texas A&M University (Prof. Perla Balbuena)		
Oakridge National Laboratory (Dr. Gergely Nagy)		
Conamix Inc. (Dr. Charlotte Hamilton)		

Project Objective
Develop new electrolytes, additives and electrode compositions for Li-S battery with high ion-conductivity, stable towards polysulfide, and promoting the polysulfide affiliation with the electrode substrate to prevent polysulfide dissolution, and enabling dendrite-free lithium metal deposition.

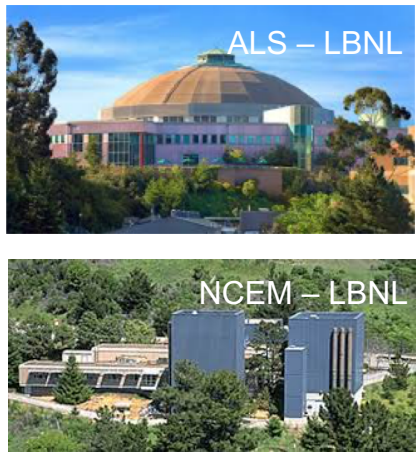
Project Impact
To address the high cost and low energy-density of the Li-ion rechargeable batteries. The emerging Li-S batteries could be both high energy-density and low cost. This project enables the applications of low cost and abundant sulfur element as a major chemical component for electrical energy storage. This project will develop new approaches for electrolytes and electrode compositions of Li-S rechargeable batteries.

Approaches

Evaluate amphiphilic fluorinated new electrolytes for Li-S rechargeable battery. Use material design and synthesis, and materials engineering to develop improved electrolytes, sulfur cathodes and lithium metal anodes. Use advanced diagnostics such as synchrotron based X-ray diffractions, electron microscopy and battery testing to characterize the Li-S materials and systems.

1. Evaluate amphiphilic fluorinated new electrolytes and additives for Li-S battery. The properties of the ideal electrolytes for sulfur electrode would be high ion conductivity, be stable towards polysulfides, and can promote the polysulfides affiliation with the electrode substrate to prevent polysulfide dissolution.
2. Chemically modify the structures of the additives, electrolyte solvents and salts to increase electrolyte stability and ionic conductivity and to prevent polysulfide dissolution and promote polysulfides precipitation.
3. Use polymer composite technology to engineer the composite sulfur cathode and lithium anode to control ion transport in both the electrolyte and the electrodes.
4. Use synchrotron based X-ray diffractions to characterize the micro and nanostructure of the electrolyte, and use electron microscopy to characterize the morphology of the electrode.
5. Use classic electrochemical testing methods to characterize the Li-S battery performance based on this new class of electrolytes.

This work is in collaboration with the LBNL synchrotron facility - the Advanced Light Source to continue our effort to develop Li-S in situ electrochemical cell for the analysis of polysulfides dissolution and precipitation during electrochemical processes; and in collaboration with the LBNL National Center for Electron Microscopy to understand the micro and nanostructure transformations in Li-S chemistry.



Accomplishments

Milestones

FY2021

1. Measure the polysulfide dissolution in the new amphiphilic electrolytes. (Completed)
2. Map out the lithium ion diffusion path in sulfur materials. (Completed)
3. Develop optimized sulfur electrodes according to the electrolyte properties and lithium ion transport in sulfur materials. (Completed)
4. Investigate the lithium metal electrode properties in the Li-S cell. (Completed)

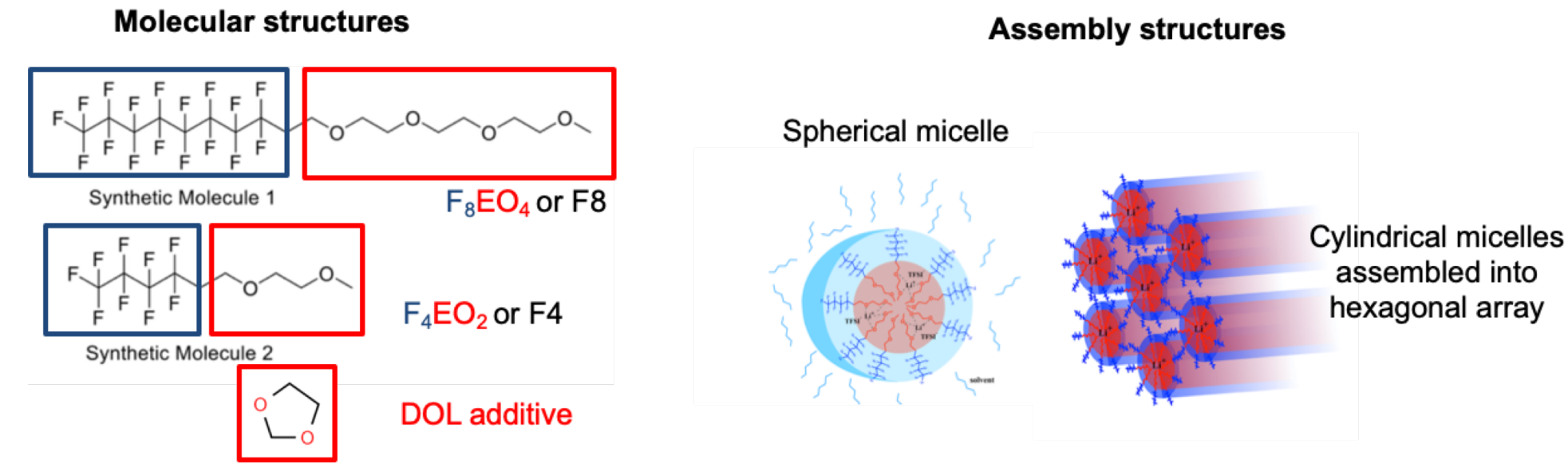
FY2022

1. Synthesize and formulate amphiphilic electrolytes using combination solvents, salts and ionic liquids. (Q1, completed)
2. Sulfur positive electrode optimization to balance ionic and electronic conductivity, as well as dissolution and precipitations properties. (Q2, completed)
3. Implement at least one strategy to stabilized Li metal anode electrode. (Q3, on-going)
4. Combine the electrolyte, sulfur electrode, and Li metal stabilization strategies to achieve stable cell cycling. (Q4, not-yet-start)

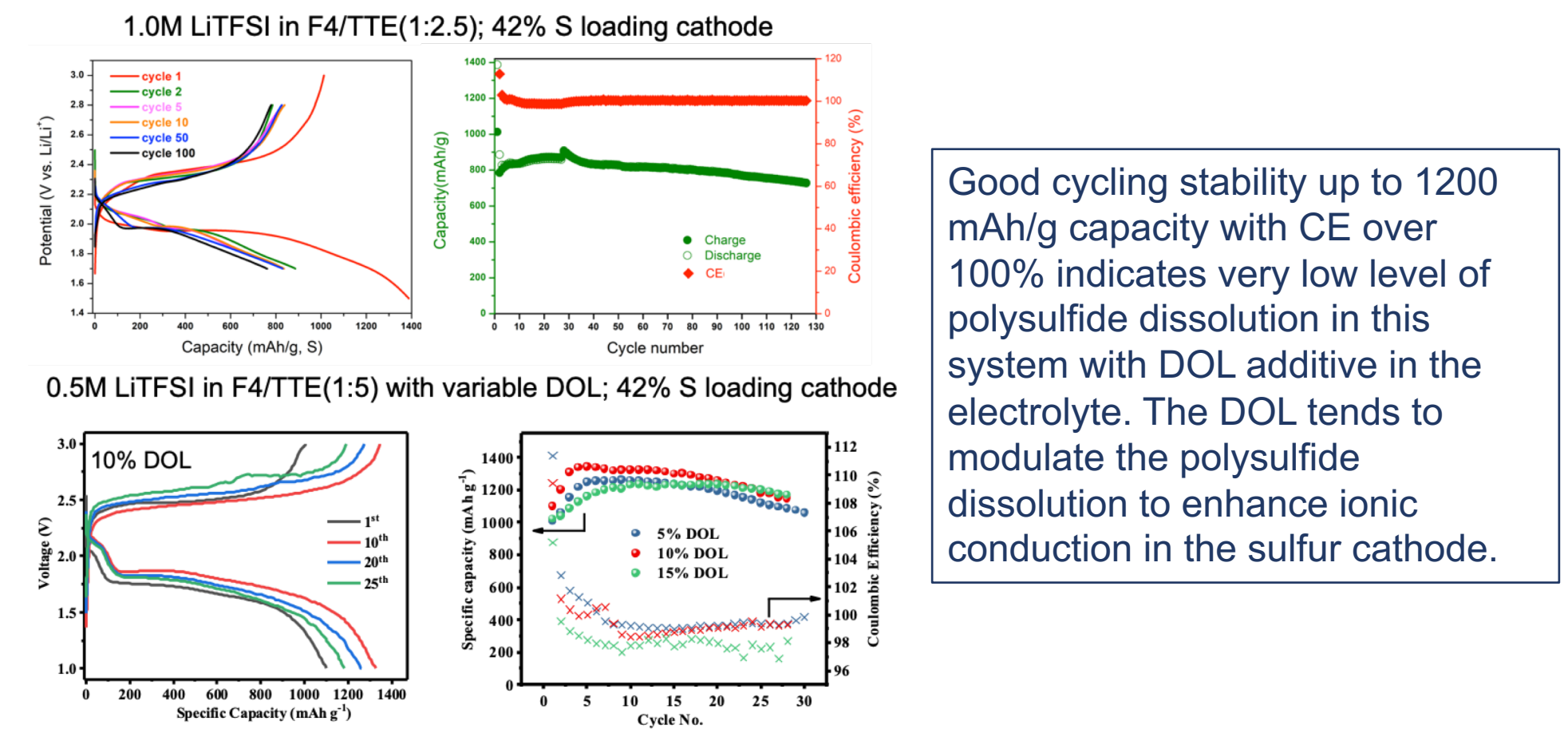
Amphiphilic fluorinated additives in hydrofluoroether (HFE) solvents

Amphiphilic fluorinated additives: Bi-functional structure of **lithiophilic head** (EO) and **lithiophobic** tail (fluorocarbon) in a HFE solvent-1,1,2,2-Tetrafluoroethyl-2,2,3,3-Tetrafluoro-propyl Ether (TTE) to improve the over all performance of the Li-S battery in all the three following aspects.

1. Electrolyte: Solvation mechanism based on micelle formation
2. Sulfur cathode: Polysulfide suppression in HFE solvents
3. Lithium metal anode: Li metal stabilization in HFE solvents

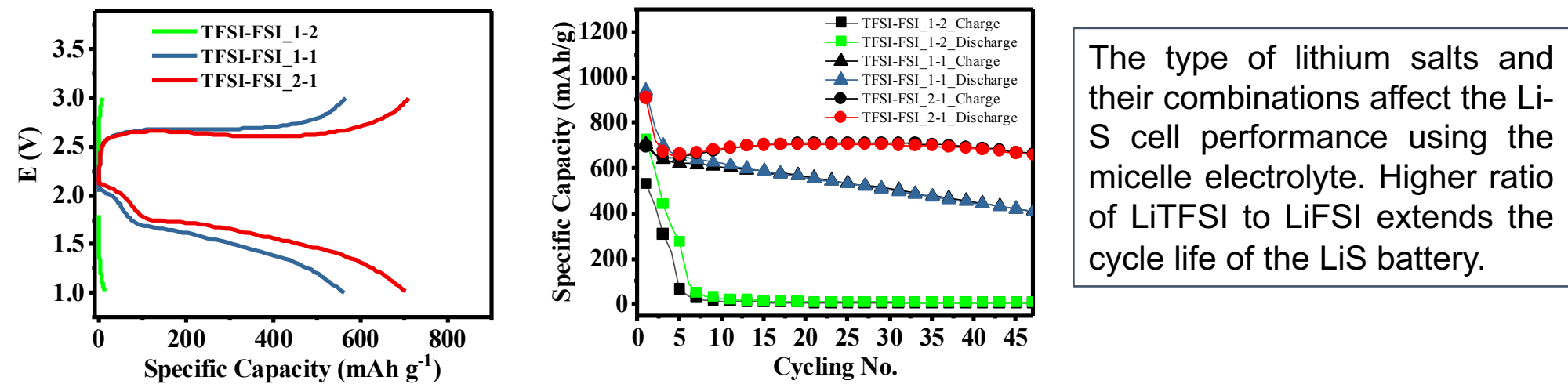


DOL lithophilic additive to the micelle electrolytes



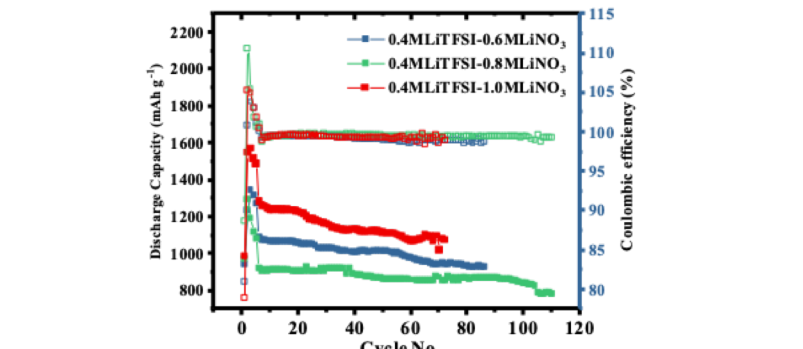
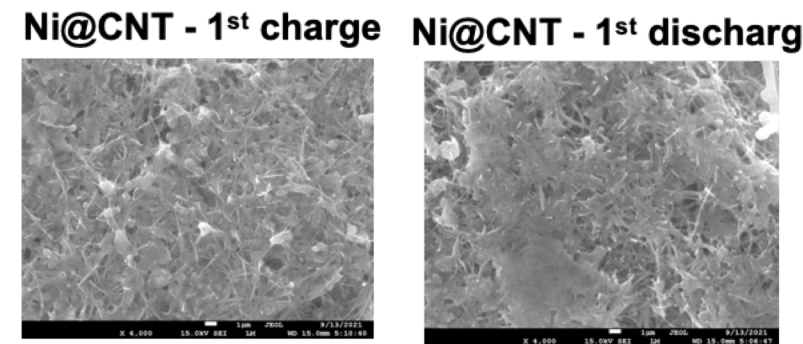
Accomplishments

Combination salts to the micelle electrolytes

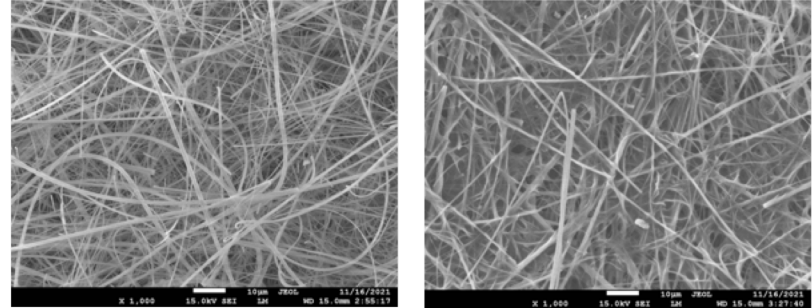
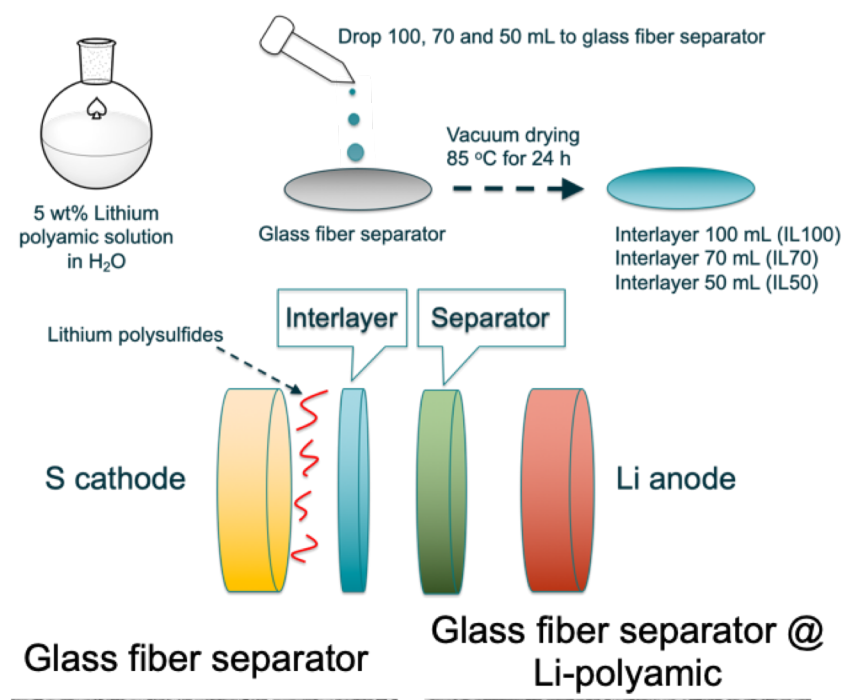


Sulfur cathode electrode and interlayer design

3D CNT-Ni form electrode to facilitated ion and electron transport

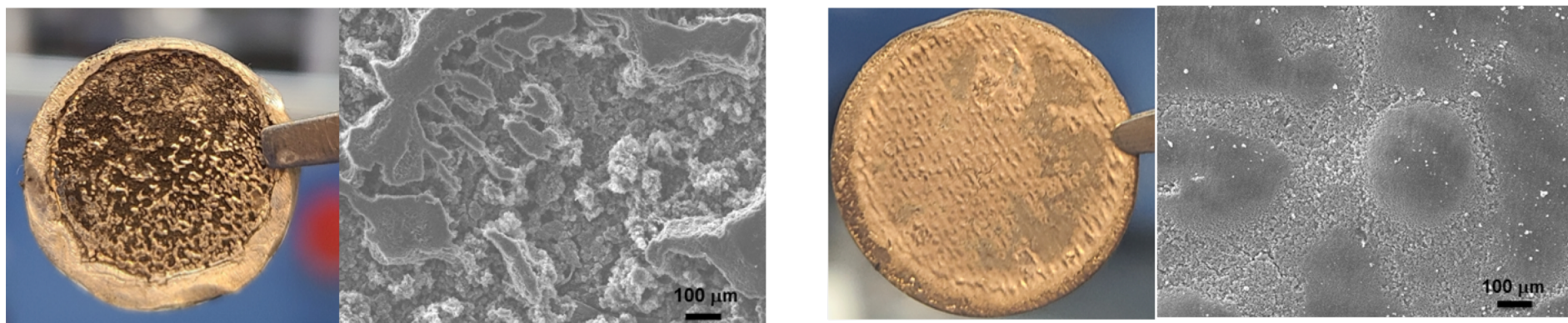


Interlayer approach to stabilized cathode

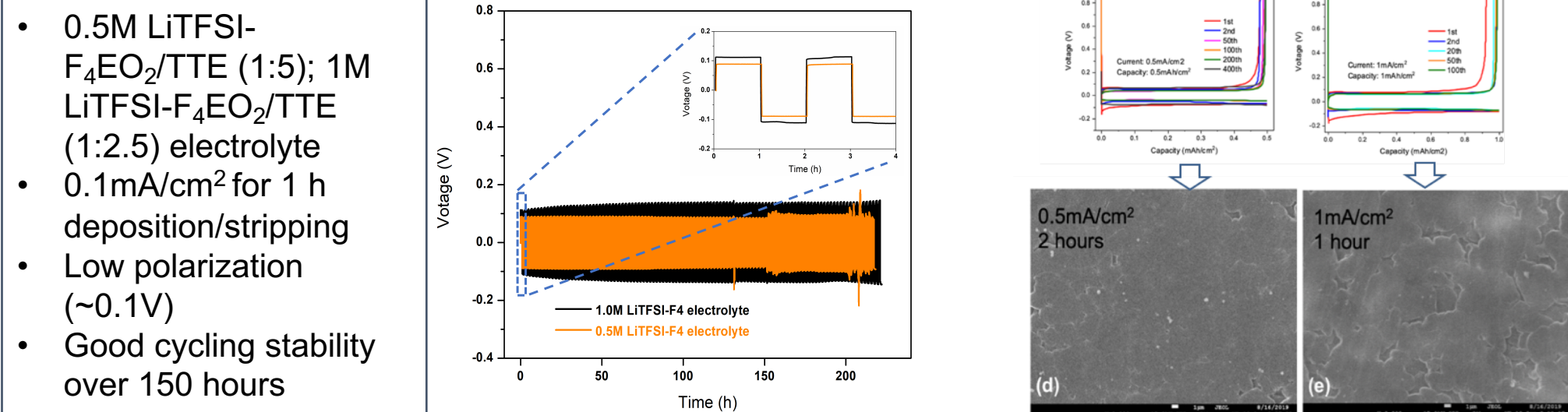


Lithium metal electrode performance

Cycled lithium metal electrode surface



Amphiphilic micelle electrolytes improve lithium deposition



Collaboration & Coordination

1. Lawrence Berkeley National Laboratory

In collaboration with synchrotron physicists Dr. Chenhui Zhu, Dr. Jinghua Guo and Dr. Wanli Yang to develop in situ cells in the beamline for the X-ray characterization to quantify the electrolyte micelle structures, polysulfide dissolution and precipitation.

2. UC Berkeley

In collaboration Prof. Andrew Minor to characterize the sulfur electrode 3D structure before and after cycling. We will use FIB and lift-out technology to prepare the cross-section of the composite electrode, and use TEM and SEM to analyze the micro and nanostructures.

3. Oak Ridge National Laboratory

In collaboration with Dr. Gergely Nagy at the Neutron Scattering Facility to character micro and nanostructures of the electrolytes. A proof-of-concept proposal was developed and approved. A full user proposal is currently under development.

4. Texas A&M University

Prof. Perla Balbuena's group conducts simulation on the polysulfide interaction with the electrode matrix in the new electrolyte. One of her students took a 3-month-stint in my group at Berkeley Lab to learn experimental details of Li-S battery. Prof. Balbuena is a BMR PI.

5. General Motors

General Motors will provide cell testing to verify the Li-S performance. GM is a partner of the VTO funded institution.

6. Conamix Inc.

Conamix is a sulfur cathodes materials solution startup company. Conamix is testing the amphiphilic electrolytes developed at Berkeley Lab.

Summary & Future Work

- Utilized amphiphilic fluorinated additives, hydrofluoroether solvents, and lithium salts based new electrolytes for Li-S battery.
- Developed and implemented diffraction characterization techniques to characterize the micelle solvation mechanism of the electrolyte.
- Characterized the polysulfides dissolution in the amphiphilic micelle electrolytes.
- Identified F₄EO₂:TTE and F₃EO₂:TTE electrolyte exhibiting superior cycling stability and high coulombic efficiency in both Li-Li cells and Li-S cells, and implemented a mixed DOL approach to improve performance.
- Implemented a cathode mesh current collector and interlayer strategy to enhance sulfur area loading.
- Future work is planned for further characterization of the new electrolytes as well as the S and Li electrodes after cycling in this new class of electrolytes, and develop Li metal surface stabilization strategy.

Future Work of Milestones for FY 2023 (Subject to change based on funding levels)

1. Measure the structure properties of the electrolytes using X-ray and neutron diffraction methods.
2. Measure the transport properties of the new electrolytes.
3. Further optimize the sulfur cathode electrode via materials synthesis and engineering to ensure sulfur cathode longevity.
4. Develop new polymer based lithium metal interface protections to prevent lithium dendrite formation. Go/No-Go: cycling lifetime at 300 cycles at over 1200 mAh/g-S utilization.

This presentation does not contain any proprietary, confidential, or otherwise restricted information.